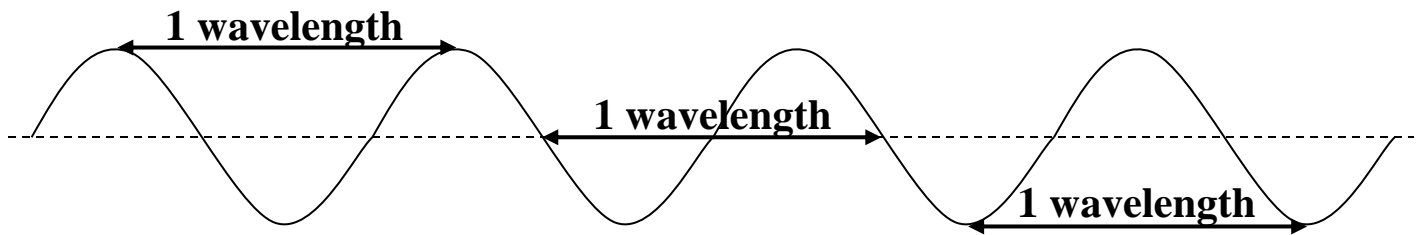


Chapter-6

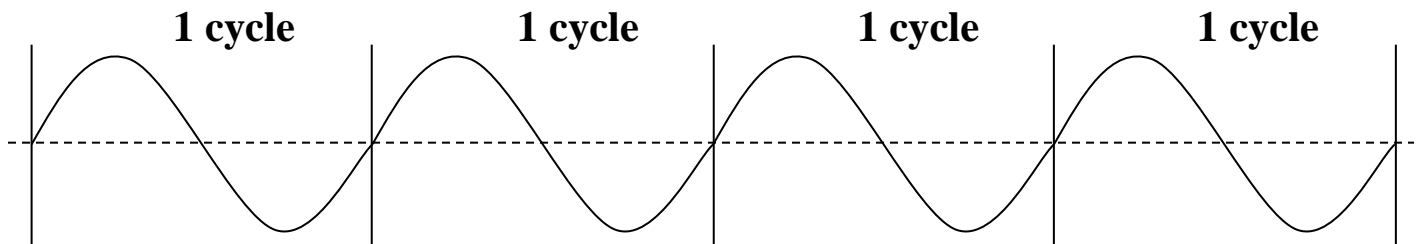
Lesson-1

I – The Wave Nature of Light

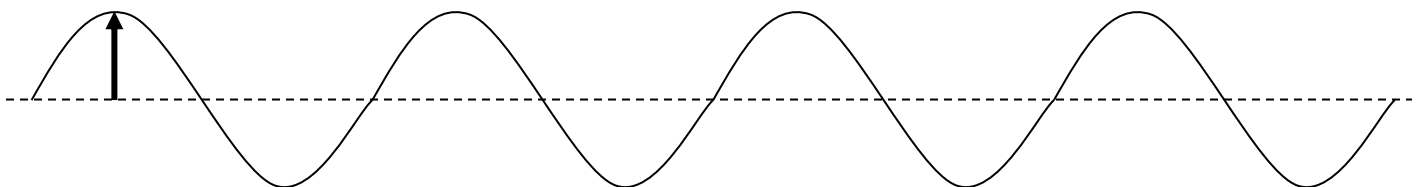
- Electromagnetic radiation (radiant energy), also known as light, is the form of energy that travels in a vacuum at 2.998×10^8 m/s.
- Electromagnetic radiation has wave characteristics.
- A wave's wavelength is the distance between two adjacent peaks (or two adjacent nodes or two adjacent troughs).



- A wave's frequency is the number of complete wavelengths (or cycles) that pass a given point each second. [frequency = cycles per second]

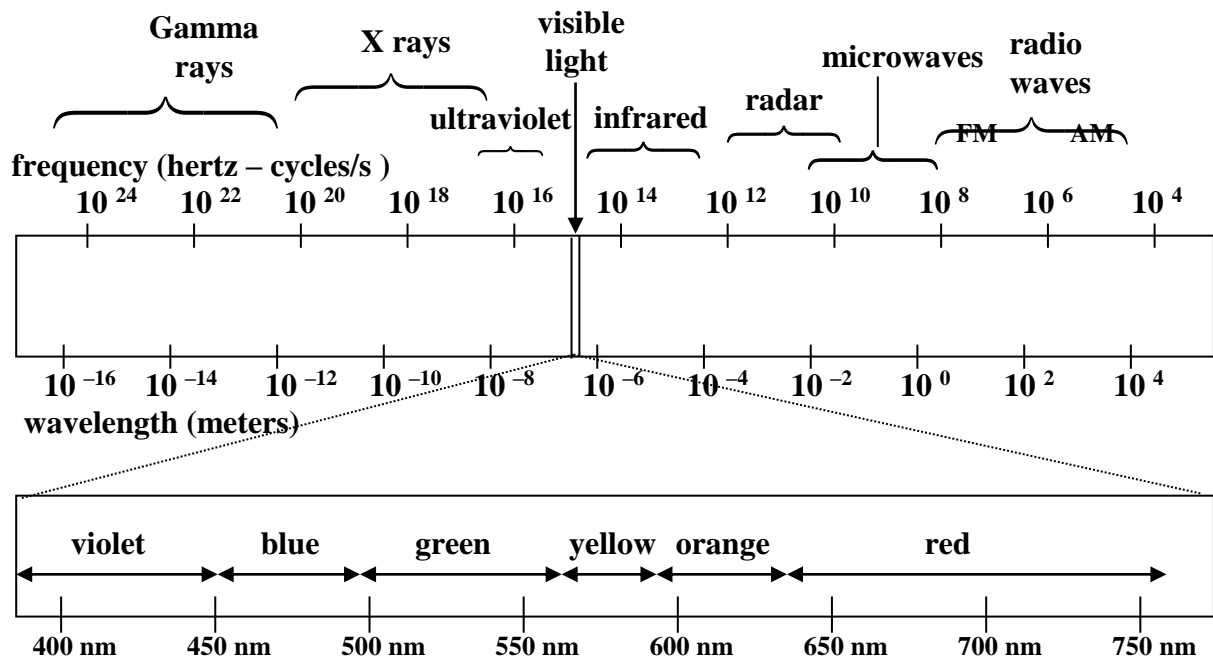


- A wave's amplitude is the maximum oscillation (height from node to peak) and is related to the intensity ("brightness") of the radiation.



A) The Relationship between Frequency & Wavelength:

- Light (electromagnetic radiation) encompasses many forms.

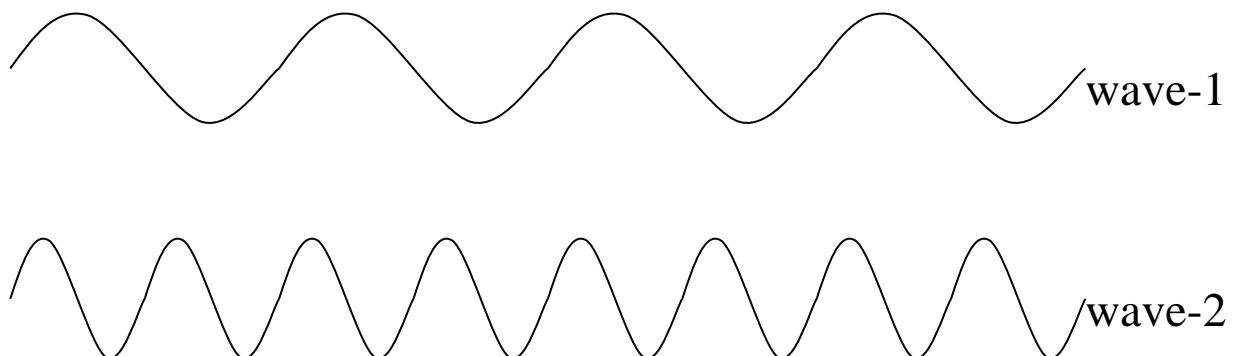


- The frequency (ν) of light is related to its wavelength (λ) by the equation:

$$c = \nu \lambda \quad \text{or} \quad \nu = c/\lambda,$$

where " ν " is the light's frequency in cycles per second (s^{-1}). The unit "cycles per second" has been given a special name, hertz (Hz). Thus, **1 Hz frequency = 1 s^{-1} frequency**.

- Below, wave-2 has twice as many cycles per unit time than wave-1, but wave-2 has half the wavelength as wave-1. Both waves have the same amplitude.



B) The Relationship between Color & Wavelength:

- Visible light has wavelengths from 400 nm (violet) to green (500 nm) to orange (600 nm) and then to 750 nm (red).
- In order for a material to have color it must absorb visible light. A material will absorb visible radiation when that radiation possesses the energy to move an electron from its ground state to some excited state.
- When a material absorbs visible light, the color we perceive is the sum of the remaining colors that are reflected or transmitted.
- When a material absorbs no visible light, the color we perceive is white and when a material absorbs all wavelengths of visible light, the color we perceive is black.

II – The Particle Nature of light

A) Postulates of Planck's Quantum Theory:

- When a system (or any of its components) can only exist in certain discrete energy states, then the system is said to be **quantized**.

*Electrons in atoms are quantized. They can only "possess" certain amounts or states of energy (**E**).*

- When a quantized system changes its energy state, it must absorb or emit **quanta of energy** that exactly corresponds to the difference between the final and initial energy states.

*Atoms absorb or release energy in discrete "chunks" called **quanta**. (ΔE)*

$$\Delta E = E_f - E_i$$

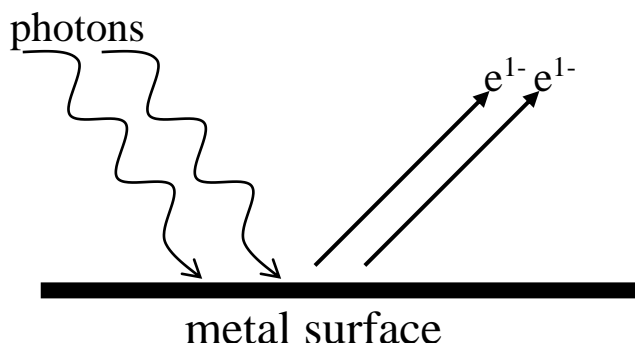
- Planck defined a **quantum of energy** as the smallest amount of energy that can be absorbed or released as radiation (light).
- Planck proposed that the energy of a single quantum of light is equal to a constant, Planck's constant (**h**), times the frequency of the radiation (**v**)

$$E = h\nu \quad (h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s})$$

B) The Photoelectric Effect and Photons:

- Einstein used Planck's quantum theory to explain the photoelectric effect.

When light with sufficient frequency strikes the surface of a metal, electrons are emitted from the metal.



- Einstein proposed that the radiant energy striking the metal surface behaved not like a wave but instead like a stream of tiny energy particles. Each radiant energy particle is called a **photon**.
- When **one photon** of minimum sufficient energy (called the “*work function*”) strikes the metal, **one electron** is emitted. If the photon's energy is greater than the minimum, then the excess energy increases the kinetic energy of the emitted electron. If the photon's energy is less than the minimum, then no electron is emitted from the metal's surface!
- Einstein deduced that each photon must have energy equal to its frequency times Planck's constant.

$$E = h\nu \quad (h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s})$$

Thus, radiant energy itself is quantized!

- Electromagnetic (E-M) radiation has particle characteristics as well as wave characteristics. Light has a wave-particle duality.

Q1: When you bite down on a wintergreen lifesaver, light is emitted in a broad band from 400 nm to 500 nm with a peak wavelength of 450 nm. In what region of the E-M spectrum is this?

A1: Visible light (blue).

Q2: What is the wavelength (in **nm**) of a photon of light whose frequency is $2.68 \times 10^{15} \text{ s}^{-1}$?

A2: $v = c/\lambda$

$$2.68 \times 10^{15} \text{ s}^{-1} = (2.998 \times 10^8 \text{ m/s}) \div (\lambda)$$

$$\boxed{\lambda = 1.12 \times 10^{-7} \text{ m} \rightarrow 112 \text{ nm}} \quad (1 \times 10^9 \text{ nm} = 1 \text{ m})$$

Q3: What is the energy of the electromagnetic radiation whose frequency is 680. kHz?

A3: $E = h\nu$

$$E = (6.626 \times 10^{-34} \text{ J}\cdot\text{s})(680. \times 10^3 \text{ s}^{-1}) = \boxed{4.51 \times 10^{-28} \text{ J}}$$

Q4: What is the energy of a photon of infrared light with a wavelength of 825nm?

A4: $E = hc/\lambda$

$$E = \frac{[(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(2.998 \times 10^8 \text{ m/s})]}{(825 \times 10^{-9} \text{ m})} = \boxed{2.41 \times 10^{-19} \text{ J}}$$

Q5: What is the energy (in **kJ/mole**) of a mole of photons whose wavelengths are 825nm? [see question #4]

$$\textbf{A5: } E = (2.41 \times 10^{-19} \text{ J})(6.022 \times 10^{23} / \text{mol}) = 145000 \text{ J/mol} \rightarrow \boxed{145 \text{ kJ/mole}}$$

Q6: Chlorophyll-a absorbs strongly in the visible spectrum at both 4400 Å and 6700 Å. FYI ... 1 Å (angstrom) in length is equal to 0.1 nm

(a) What “colors” does chlorophyll-a absorb from the visible spectrum?

(b) What color is chlorophyll-a?

A6: (a) **VIOLET-BLUE @ 440 nm & ORANGE-RED @ 670 nm**
(b) **GREEN – of course!**

Q7: What is the frequency (in **MHz**) of a photon of infrared light whose wavelength is 825nm? [*M is the prefix mega = 1×10^6*]

A7: $v = c/\lambda$

$$v = \frac{2.998 \times 10^8 \text{ m/s}}{825 \times 10^{-9} \text{ m}} = 3.63 \times 10^{14} \text{ s}^{-1} \rightarrow 3.63 \times 10^{14} \text{ Hz}$$

$$3.63 \times 10^{14} \text{ Hz} \times \frac{1 \text{ MHz}}{1 \times 10^6 \text{ Hz}} = \boxed{3.63 \times 10^8 \text{ MHz}}$$

Q8: It has been determined that a single gaseous iodine molecule (I_2) will separate into individual gaseous iodine atoms ($\rightarrow \text{I} + \text{I}$) after the absorption of light with wavelengths less than 499.5 nm. What is the minimum amount of energy in joules that would decompose a single iodine molecule?

A8: $E = hc/\lambda$

$$E = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s})(2.998 \times 10^8 \text{ m/s})}{(499.5 \times 10^{-9} \text{ m})} = \boxed{3.977 \times 10^{-19} \text{ J}}$$

Q9: What is the amount of energy needed to decompose iodine molecules in kJ/mol?

$$\textbf{A9: } E = (3.977 \times 10^{-19} \text{ J}) \times \frac{(1.00 \text{ kJ})}{1000 \text{ J}} \times \frac{(6.022 \times 10^{23})}{1.00 \text{ mole}} = \boxed{239.5 \text{ kJ/mol}}$$

Q10: One of the green spectral lines in the emission spectra of neon has a wavelength of 480. nm. Calculate the energy of the photon being emitted.

A10: $E = hc/\lambda$

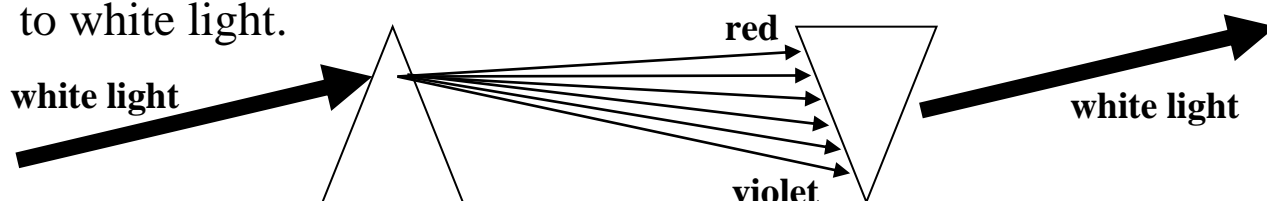
$$E = \frac{(6.626 \times 10^{-34} \text{ J s})(2.998 \times 10^8 \text{ m/s})}{(480. \times 10^{-9} \text{ m})} = \boxed{4.14 \times 10^{-19} \text{ J}}$$

Chapter-6

Lesson-2

III The Bohr Model of the Atom

- In 1665, Newton discovered that white light is composed of the colors of the rainbow (ROYGBV) by passing a beam of white light through a prism and then passing the resultant beam of refracted light through a second prism which then recombined to white light.



- In 1859, the spectroscope was introduced by Bunsen and Kirchoff and they, and others, used the unique line spectra seen within to identify known elements and to discover new elements.
- In 1885, Balmer showed that the wavelengths of the four visible spectral lines of hydrogen fit the simple equation:

$$\frac{1}{\lambda} = 1.096776 \times 10^7 \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \quad \dots \text{only for the four visible spectral lines in hydrogen}$$

where the units for 1.096776×10^7 were “ m^{-1} ” and n was an integer 3, 4, 5, or 6.

- Shortly after, and independently, Rydberg introduced a general equation that related the any spectral line of hydrogen (in the *infrared*, *visible*, or *ultraviolet region*) to its wavelengths. This is known as the Rydberg equation.

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad \dots \text{for any of the spectral lines in hydrogen}$$

where R_H is $1.096776 \times 10^7 \text{ m}^{-1}$ and n_1 and n_2 were positive integers, with n_2 being larger than n_1 .

- Both the Balmer and Rydberg equations were empirically derived but neither could be explained theoretically.

- In 1913, Niels Bohr advanced a theory of atomic structure that would account for the line spectra of elements and to circumvent the objections leveled against the Rutherford atom.
- Bohr postulated (#1) that electrons moved (v) about the nucleus in a circular orbit of fixed radius ($2\pi r$). He restricted the orbits for electron revolution to those for which the angular momentum (mvr) is a whole number multiple (n) of the quantity ($h/2\pi$).

$$mvr = n(h/2\pi) \quad \text{where } n = \text{the PEL \#}$$

- Bohr further postulated (#2) that as long as an electron remains in a given orbit it does not radiate energy, thus the energy of an electron remains constant. Since electron orbits are quantized (by angular momentum) and since the energy of any electrons in these orbits are constant, then the orbits represent quantized energy levels (E_n).

$$\begin{array}{l} \text{"sitting" in a PEL} \\ \text{energy} \end{array} \quad E = \frac{-2.178 \times 10^{-18} \text{ J}}{n^2} \quad \text{where } n = \text{the PEL \#}$$

This represents the energy of an electron in a particular orbit (n).

- (#3) In order for an electron to jump up from its normal orbit (ground state) in an atom to an orbit of higher energy (excited state), the electron would need to absorb the specific quantum of energy (ΔE) that was equal to the energy difference of the two orbits.

$$\begin{array}{l} \text{"jumping up"} \\ \text{energy} \end{array} \quad \begin{array}{l} \Delta E = E_{hi}^{final} - E_{lo}^{initial} \\ \Delta E = +h\nu \quad \text{or} \quad \Delta E = +hc/\lambda \end{array}$$

- Finally, Bohr stated that each line observed in the spectrum of an element resulted from the passage of an electron from an orbit of higher energy (E_{hi} - excited state) to an orbit of lower energy (E_{lo}).

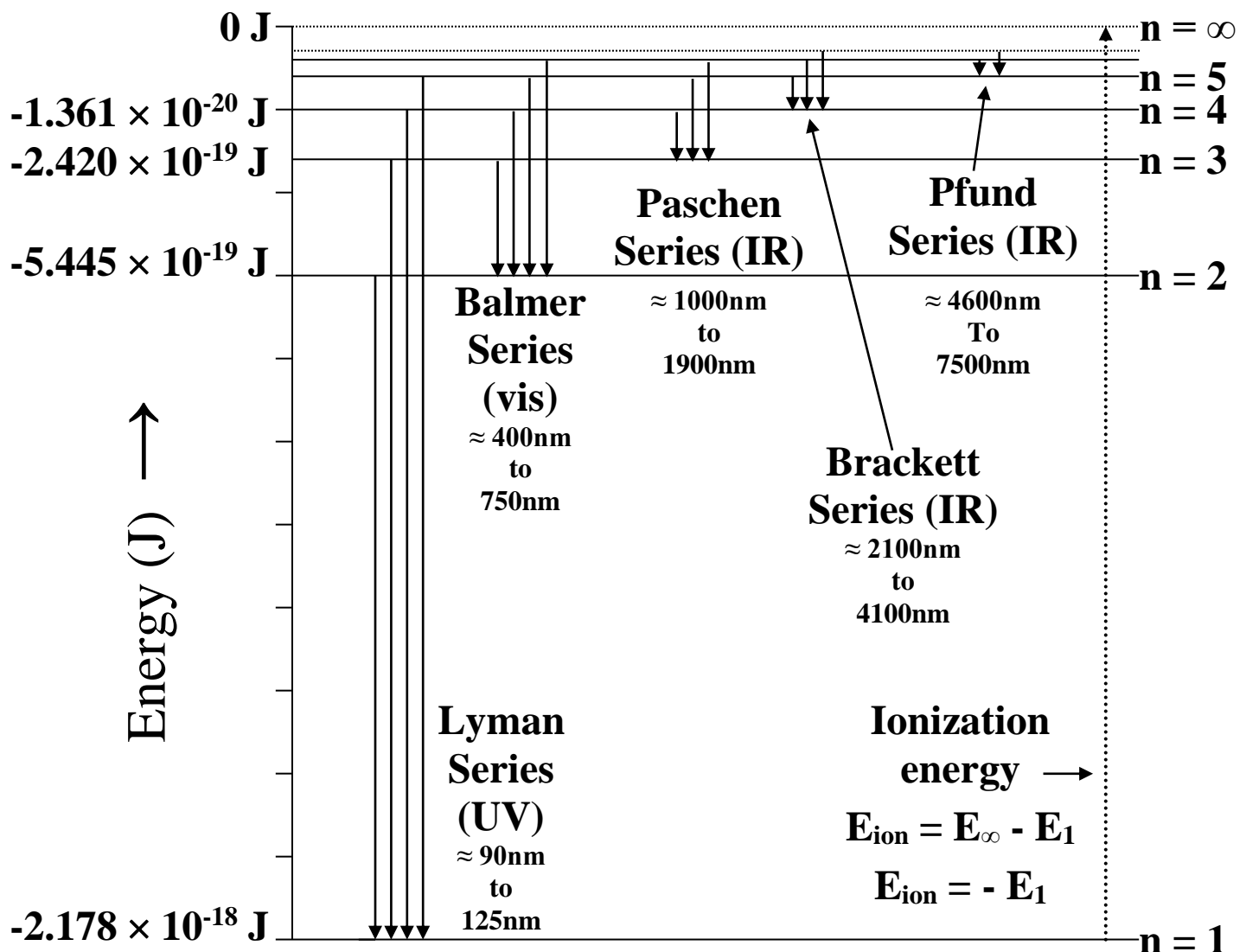
$$\begin{array}{l} \text{"jumping down"} \\ \text{energy} \end{array} \quad \begin{array}{l} \Delta E = E_{lo}^{final} - E_{hi}^{initial} \\ \Delta E = -h\nu \quad \text{or} \quad \Delta E = -hc/\lambda \end{array}$$

- Bohr proceeded to apply these ideas to the hydrogen atom.

- In a hydrogen atom, the single electron's ground state is the orbit of lowest energy ($n = 1$). Any energy state above the ground state ($n = 1$) is referred to as an excited state ($n = 2, n = 3, \dots, n = n$). The energies of the electron of a hydrogen atom are negative for all values of n . The lower (more negative) the energy is, the more stable the atom will be.
- When n is equal to ∞ , the electron has "left the atom"! In a hydrogen atom, the energy needed to completely separate the electron from the proton is assigned a value of $2.178 \times 10^{-18} \text{ J}$ per electron (1312 kJ per mole of electrons).

$$\Delta E = - 2.178 \times 10^{-18} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \quad \text{"Jumping" energy}$$

where n_i is the initial PEL and n_f is the final PEL



Q1: What is the ionization energy for a ground state hydrogen atom in kJ/mol?

A1: $E_{\text{ion}} = \Delta E_{\text{absorbed}} = -2.178 \times 10^{-18} \text{ J } (1/n_f^2 - 1/n_i^2)$

$$E_{\text{ion}} = (-2.178 \times 10^{-18} \text{ J})(-1/n_i^2) \leftarrow [\text{since } n_f = \infty, \text{ then } 1/n_f^2 = 0]$$

$$E_{\text{ion}} = -(-2.178 \times 10^{-18} \text{ J}) \left(\frac{1}{1^2} \right) \left(\frac{1 \text{ kJ}}{1000 \text{ J}} \right) \left(\frac{6.022 \times 10^{23}}{1 \text{ mol}} \right)$$

$$E_{\text{ion}} = 1312 \text{ kJ/mol}$$

Q2: What is the wavelength of light (photon) emitted when the excited electron in a hydrogen atom jumps from the 3rd orbit to the 2nd orbit?

A2: $\Delta E = -2.178 \times 10^{-18} \text{ J } (1/n_f^2 - 1/n_i^2)$

$$\Delta E = -2.178 \times 10^{-18} \text{ J } (1/2^2 - 1/3^2)$$

$$\Delta E = -3.025 \times 10^{-19} \text{ J}$$

$$\Delta E = -hc/\lambda$$

$$-3.025 \times 10^{-19} \text{ J} = [-(6.626 \times 10^{-34} \text{ J s})(2.998 \times 10^8 \text{ m/s})]/\lambda$$

$$\lambda = 6.567 \times 10^{-7} \text{ m} \quad \text{or} \quad 656.7 \text{ nm} \quad \text{FYI, it looks orange-red}$$

Q3: A spectral line in the hydrogen atom has a wavelength of 485 nm. From what higher orbit (energy level) did the electron jump?

A3: $\Delta E = -hc/\lambda$

$$\Delta E = [-(6.626 \times 10^{-34} \text{ J s})(2.998 \times 10^8 \text{ m/s})]/485 \times 10^{-9} \text{ m}$$

$$\Delta E = -4.10 \times 10^{-19} \text{ J}$$

$$\Delta E = -2.178 \times 10^{-18} \text{ J } (1/n_f^2 - 1/n_i^2)$$

$$-4.10 \times 10^{-19} \text{ J} = -2.178 \times 10^{-18} \text{ J } (1/2^2 - 1/n_i^2)$$

$$-4.10 \times 10^{-19} \text{ J} = -5.445 \times 10^{-19} \text{ J} + 2.178 \times 10^{-18}/n_i^2$$

$$1.35 \times 10^{-19} \text{ J} = 2.178 \times 10^{-18} \text{ J}/n^2$$

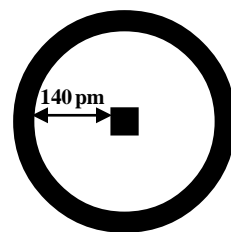
$$n = 4 \quad \text{or} \quad \text{the 4}^{\text{th}} \text{ orbit (energy level)}$$

Chapter-6

Lesson-3

IV – The Quantum Mechanical Model of the Atom

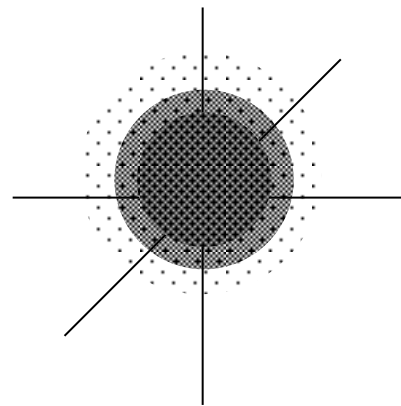
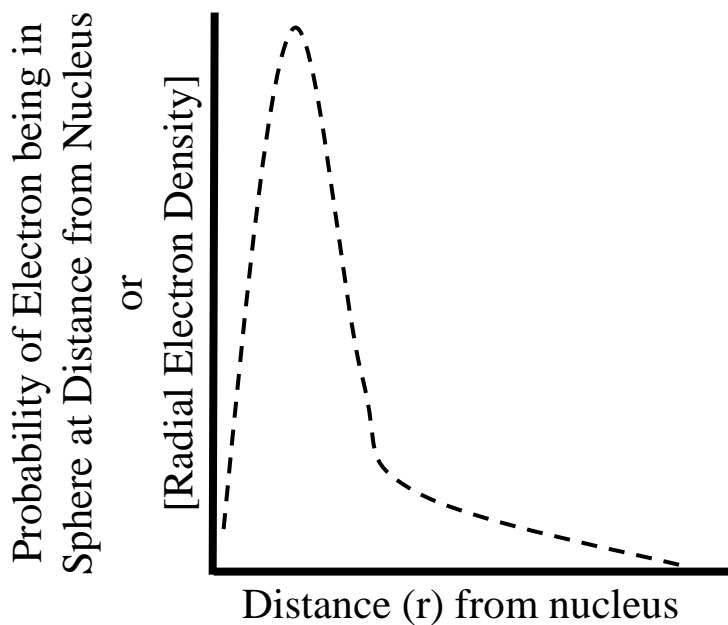
- In the 1920's a new discipline, called **quantum mechanics**, was developed to describe the motion of small particles confined in very small spaces. The primary function of quantum mechanics is to find expressions for the energies of these particles.
- In the **quantum mechanical atom**, no attempt is made to specify neither the position (at a given instant) nor the path of an electron in the atom. Instead, the electron's "position" in the atom is described as being in a location of probability.
- For example, the ground state electron in an atom of hydrogen has a 90% probability of being found at a distance of 140 pm from the nucleus in any direction.
- In 1926, Erwin Schrödinger derived an equation that is the basis for quantum-mechanical model of the hydrogen atom.



$$H\psi = E\psi$$

where ψ is the wave function of the electron's position in space, E is the total energy of the atom, and H is a set of mathematical instructions called an operator.

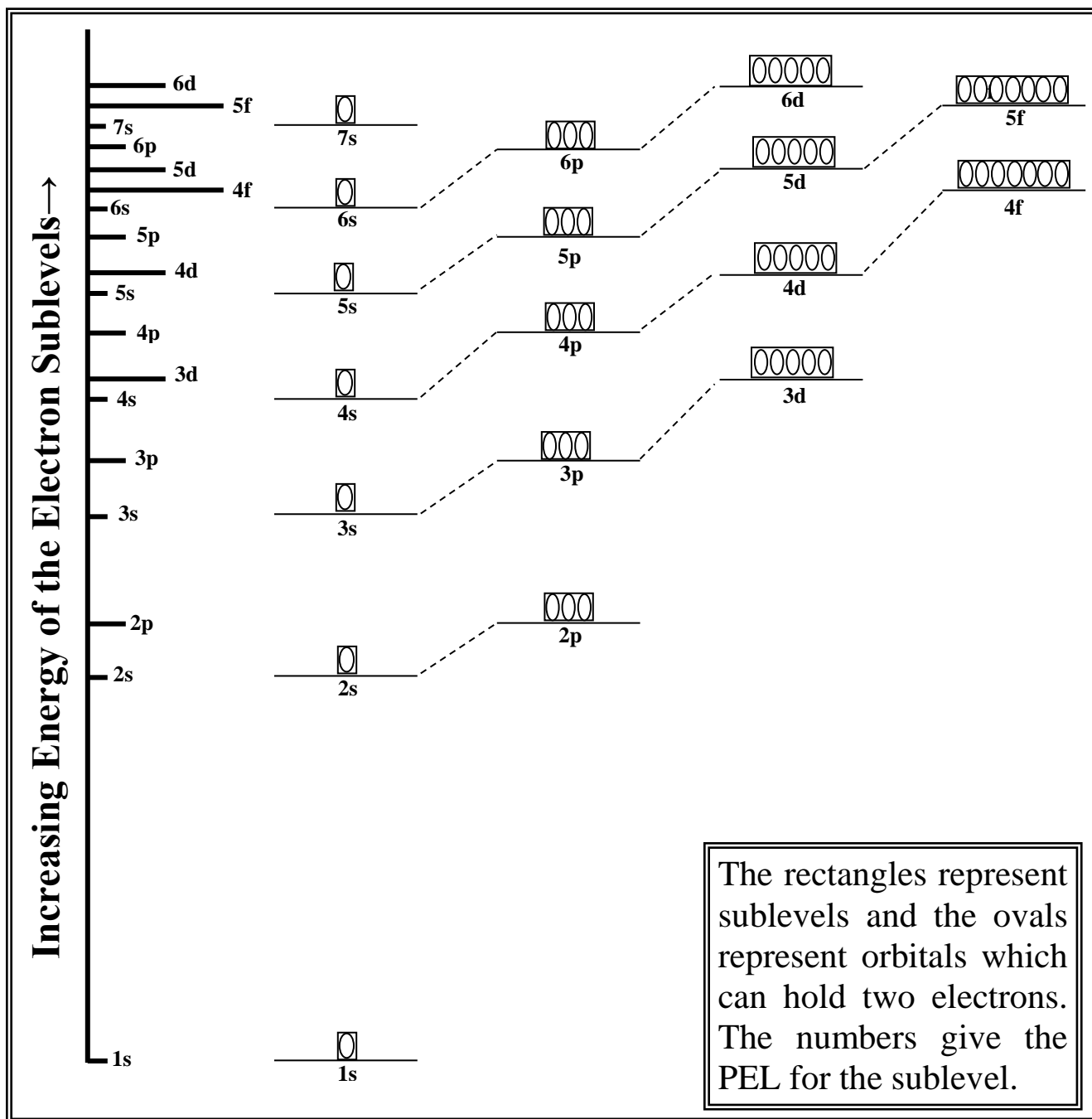
- There are many solutions for this equation. Each solution consists of a wave function (ψ) which is characterized by a specific value of E (energy).
- A specific wave function is called an **orbital**.
- *Each wave function (ψ) itself has no direct physical meaning.*
- The square of the wave function (ψ^2), however, is directly proportional to the probability of finding the electron at that point. Thus ψ^2 is proportional to the **electron cloud density** or the **probability density**.
- Therefore each orbital has a characteristic **energy** and **shape**.



Electron density distribution in a ground state hydrogen atom

A) Orbital Energies:

- Electrons are “found” outside the atom’s nucleus in various principle energy levels (PELs). **1st PEL, 2nd PEL, 3rd PEL, etc.**
- Within an atom, the PEL energies increase: **1st → 2nd → 3rd → ...**
- Within each PEL, electrons are “found” in energy sublevels.
 - The **1st PEL** has one energy sublevel: **s**
 - The **2nd PEL** has two energy sublevels: **s p**
 - The **3rd PEL** has three energy sublevels: **s p d**
 - The **4th PEL** has four energy sublevels: **s p d f**
 - The **5th PEL** has five energy sublevels: **s p d f g**
- Within a PEL, sublevel energies increase: **s → p → d → f → ...**
- Within each energy sublevel, electrons are “found” in orbitals.
 - The **s-sublevel** has one orbital: **s**
 - The **p-sublevel** has three orbitals: **p_x p_y p_z**
 - The **d-sublevel** has five orbitals: **d_{xy} d_{xz} d_{yz} d_{x²-y²} d_{z²}**
 - The **f-sublevel** has seven orbitals: **f f f f f f f**
 - The **g-sublevel** has nine orbitals: **g g g g g g g g g**
- Within an energy sublevel, the orbitals all have equal energy!



Q3: Which of the following are possible energy sublevels for an electron? (a) 4s (b) 2d (c) 1s (d) 3f (e) 6d (f) 3p

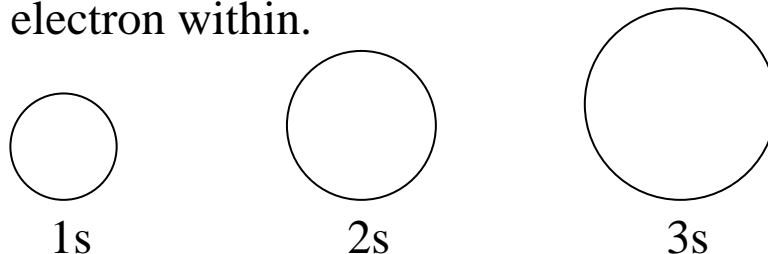
A3: (a) yes (b) no (c) yes (d) no (e) yes (f) yes

Q4: How many orbitals orientations do the following sublevels have?
(a) s (b) p (c) d (d) f

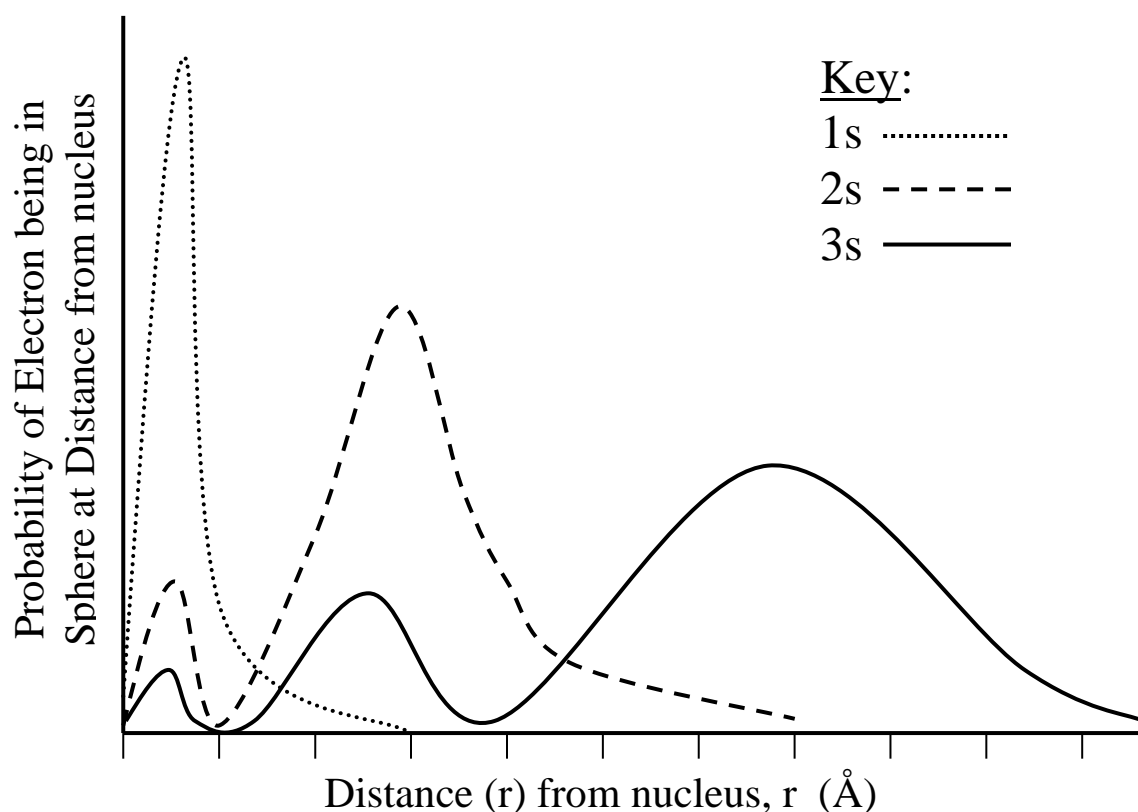
A4: (a) 1 (b) 3 (c) 5 (d) 7

B) Orbital Shapes:

- The lowest-energy orbital in every PEL is the **s-orbital**.
- The s-orbital is spherically symmetrical about the atom's nucleus.
- The contour representation of an s-orbital is a sphere. The relative radius of the sphere corresponds to a 90% probability of finding the electron within.

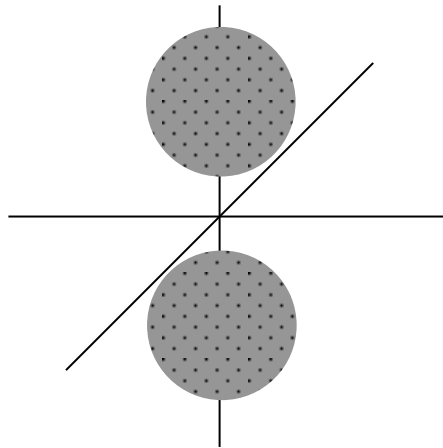


- An s-orbital can be graphically represented as a **radial probability function** which is a plot of the ***radial probability density*** as a function of the ***distance from the nucleus***.

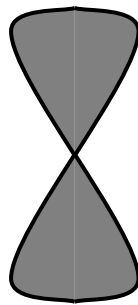


- In the quantum (wave) mechanical model, the most probable distance at which to find the electron in the 1s-orbital is 0.529 \AA . As it turns out, this is the same radius of the circular orbit (exact distance) predicted by Bohr for $n = 1$. [$1 \text{ \AA (angstrom)} = 100 \text{ pm}$]
- In the 2s and 3s orbitals **the radial probability function** drops to zero at certain distances from the nucleus and then rises again.

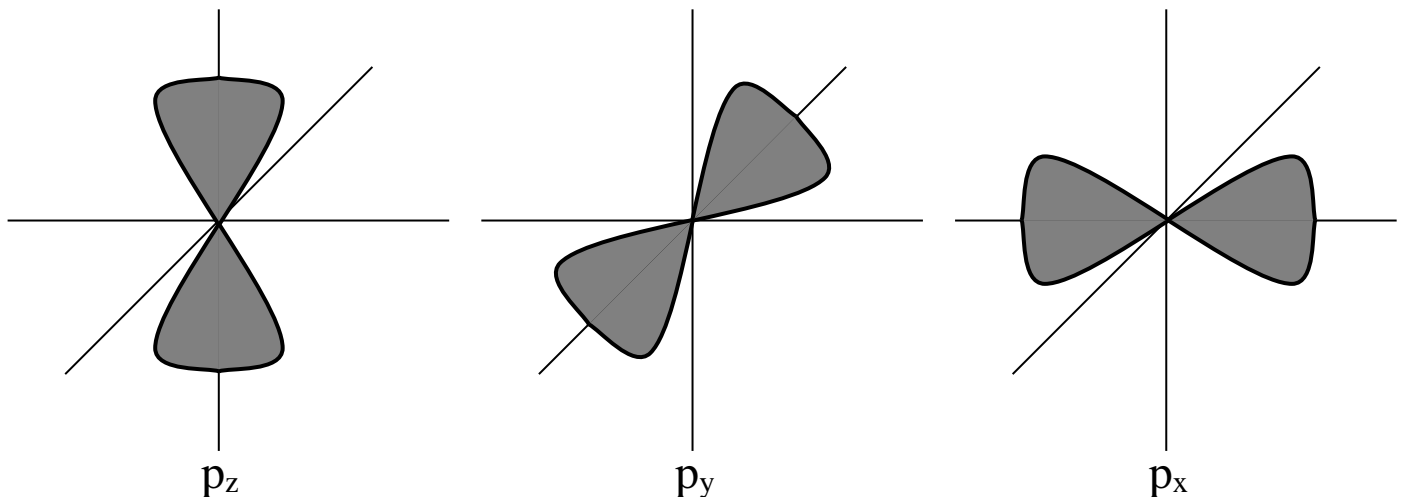
- The second level of energy orbitals in a PEL is the **p-orbital**.
- The p-orbital is dumbbell-shaped about the atom's nucleus.



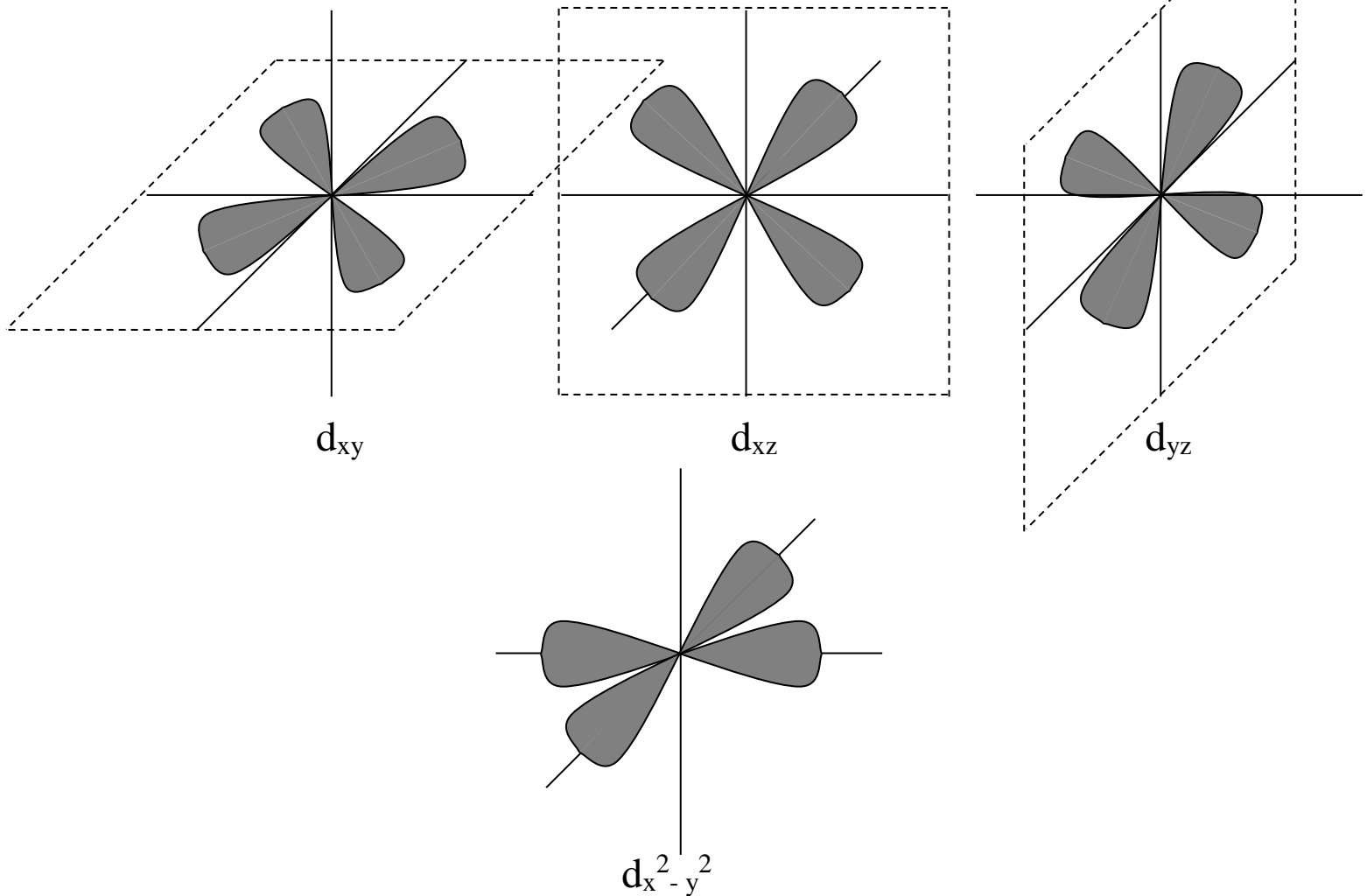
- The contour representation of p-orbital is shown below.



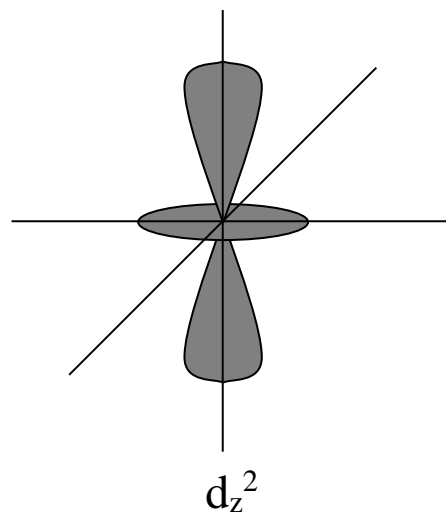
- In each PEL (*where $n = 2$ or more*) there are three p-orbitals.
- Each p-orbital is oriented perpendicularly to the other two. For convenience, the p-orbitals are labeled p_x , p_y , and p_z .
- The letter subscripts indicate the Cartesian axis along which the orbital is oriented.



- The third level of energy orbitals in a PEL is the **d-orbital**.
- In each PEL where $n = 3$ or more there are five d-orbitals.
- The contour representation for four of the d-orbitals have a “four-leaf-clover” shape as shown below.



- The contour representation for the fifth d-orbital has a “dumbbell-with-a-doughnut” shape as shown below and is oriented along the z -axis with the doughnut around the origin.



Chapter-6

Lesson-4

V – Many-Electron Atoms & Electronic Structures

There are several ways to show the electronic structure (the electron configuration) of an atom.

A) The (Sublevel) Electron Configuration:

- This model shows the number of electrons in each PEL as well as in each sublevel. This model is generically referred to as the electron configuration.
- The maximum number of electrons that each sublevel can hold is as follows:
 - the s-sublevel can hold 2 electrons
 - the p-sublevel can hold 6 electrons
 - the d-sublevel can hold 10 electrons
 - the f-sublevel can hold 14 electrons
- The problem in ordering the sublevels is that the PELs begin to overlap each other.
- The diagram at the right shows the ordering of the sublevels from lowest to highest energy.
- This is known as the **aufbau ordering principle**.

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f 5g
6s 6p 6d 6f 6g
7s 7p 7d 7f 7g
8s 8p 8d 8f 8g

Q1: What is the electron configuration for the following elements in the ground state? (a) Al _(13e⁻) (b) K _(19e⁻) (c) Cd _(48e⁻) (d) Ho _(67e⁻)

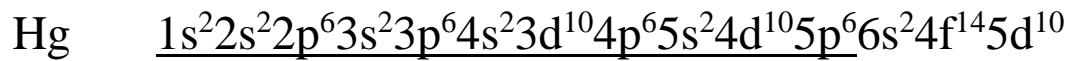
A1: (a) $1s^2 2s^2 2p^6 3s^2 3p^1$

(b) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

(c) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10}$

(d) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{11}$

- The electron configurations for large elements can get very long!



- Electron configurations for large elements can be shortened into what is called the condensed electron configurations!

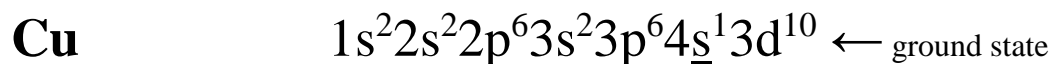
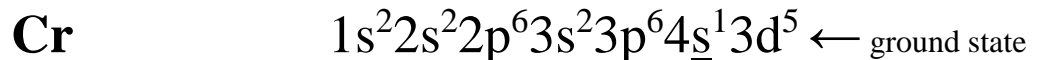


Q2: Write the condensed ground state electron configuration for (a) cadmium and (b) holmium? Consult your answers to question-1.

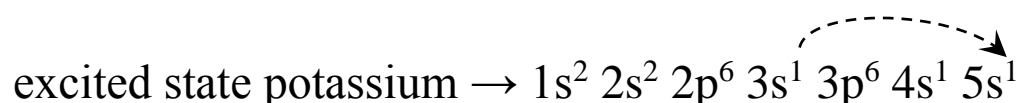
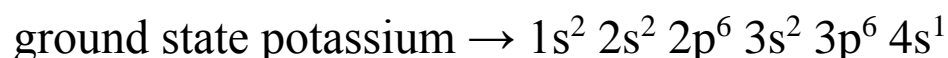
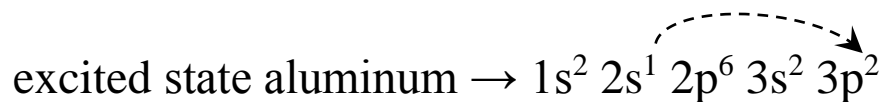
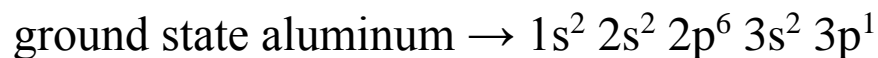


- There are exceptions to the ordering of the electrons in the ground state. Two notable exceptions are:

<u>Element</u>	<u>(sublevel) Electron Configuration</u>
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- Atoms can be found in the excited state as a result of one or more electrons having jumped to a higher energy level after having absorbed energy



B) Electron Configurations and the Periodic Table:

- The Structure of the Periodic Table of Elements directly corresponds to the electronic structure of the elements.
- The Periodic Table of Elements consists of four blocks: the s-block, the p-block, the d-block, and the f-block which corresponds to the sublevels. The “width” of each block corresponds to the maximum number of electrons allowed in each sublevel.
- An element’s location in a particular block directly corresponds to the number of electrons in the highest energy sublevel in a ground state atom of that element.

1s						1s
2s						2p
3s					Al	3p
K 4s			3d			4p
5s			4d		Cd	5p
6s			5d			6p
7s			6d			7p
<div> <div>4f</div> <div>Ho</div> </div>						
5f						

- An element’s electron configuration can be determined from its location on the Periodic Table of Elements by using the **aufbau ordering principle**.

Al $1s^2 2s^2 2p^6 3s^2 \mathbf{3p^1}$

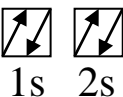
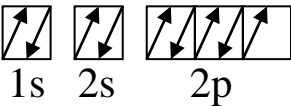
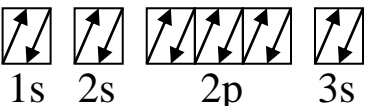
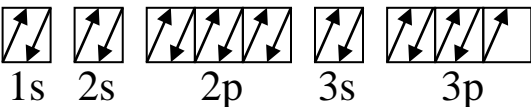
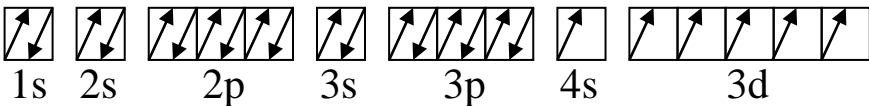
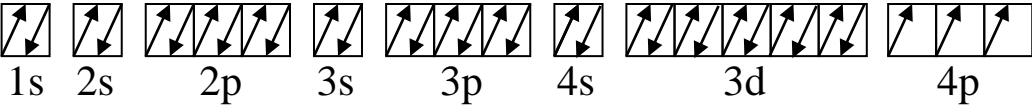
K $1s^2 2s^2 2p^6 3s^2 3p^6 \mathbf{4s^1}$

Cd $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 \mathbf{4d^{10}}$

Ho $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 \mathbf{4f^{11}}$

C) The (Orbital Diagram) Electron Configuration:

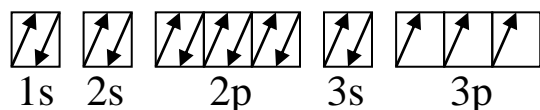
- All orbitals, no matter of size, shape, or orientation, will hold a maximum of two electrons.
- Electrons must have opposite spins when found in the same orbital. (**Pauli Exclusion Principle**)
- Orbitals in the same sublevel must each contain one electron before any orbital in that same sublevel will gain a second electron. (**Hund's Rule**)
- Orbitals in the same sublevel possess the same energy but are oriented differently in space.
- The number of orbits found in a particular sublevel is as follows:
 - the s-sublevel contains 1 orbital
 - the p-sublevel contains 3 orbitals
 - the d-sublevel contains 5 orbitals
 - the f-sublevel contains 7 orbitals

<u>Element</u>	<u>Electron configuration</u>	<u>Orbital Diagram</u>
Be	$1s^2 2s^2$	 1s 2s
F	$1s^2 2s^2 2p^5$	 1s 2s 2p
Mg	$1s^2 2s^2 2p^6 3s^2$	 1s 2s 2p 3s
Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	 1s 2s 2p 3s 3p
exception Cr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$	 1s 2s 2p 3s 3p 4s 3d
As	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$	 1s 2s 2p 3s 3p 4s 3d 4p

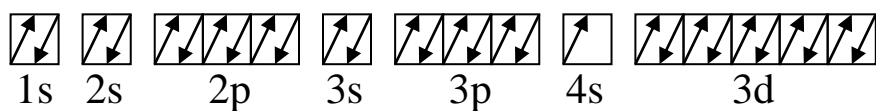
Q3: Write the full electron configuration and orbital notation for the following neutral elements in the ground state?

(a) P _(15e⁻) (b) Cu _(29e⁻)

A3: (a) $1s^2 2s^2 2p^6 3s^2 3p^3$



(b) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$



D) The (PEL) Electron Configuration:

- This model only gives the total number of electrons in each PEL of an atom. The maximum number of electrons in a particular PEL (n) is equal to **$2n^2$** .

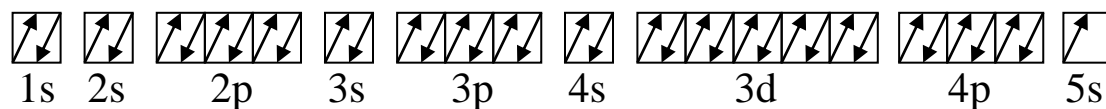
- | | |
|---|--|
| - The 1 st PEL holds up to 2 electrons. | Max #e⁻ in a PEL
=
$2n^2$ |
| - The 2 nd PEL holds up to 8 electrons. | |
| - The 3 rd PEL holds up to 18 electrons. | |
| - The 4 th PEL holds up to 32 electrons. | |

<u>Element</u>	<u>Electron Configuration</u>	<u>PEL Electron Configuration</u>
H	$1s^1$	1
He	$1s^2$	2
Li	$1s^2 2s^1$	2-1
Be	$1s^2 2s^2$	2-2
F	$1s^2 2s^2 2p^5$	2-7
Mg	$1s^2 2s^2 2p^6 3s^2$	2-8-2
P	$1s^2 2s^2 2p^6 3s^2 3p^3$	2-8-5
Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$	2-8-8
Co	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$	2-8-15-2
Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$	2-8-18-8
Zr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^2$	2-8-18-10-2
Pb	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^2$	2-8-18-32-18-4

Q4: Write the full electron configuration, the orbital notation and the PEL electron configuration for the following neutral elements in the ground state?

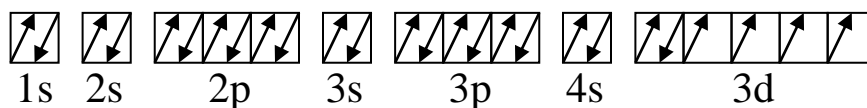
(a) Rb (b) Fe (c) Si (d) Se

A4: (a) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1$



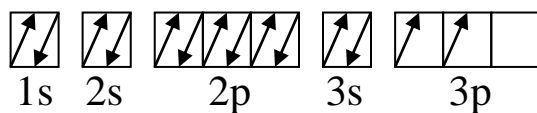
2-8-18-8-1

(b) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$



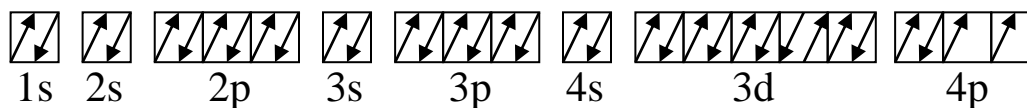
2-8-14-2

(c) $1s^2 2s^2 2p^6 3s^2 3p^2$



2-8-4

(d) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$



2-8-18-6

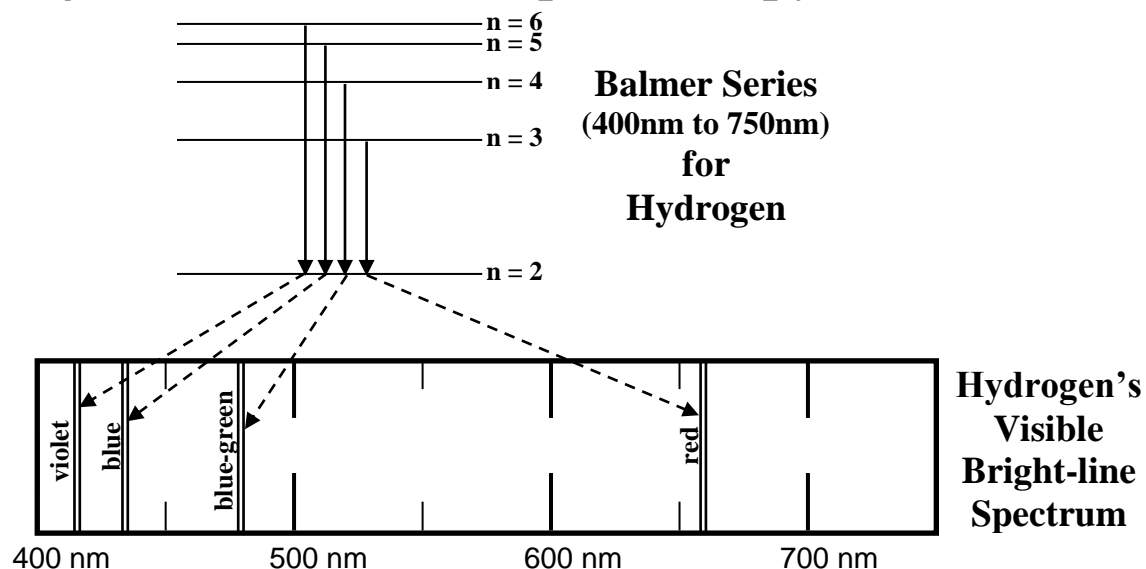
Chapter-6

Lesson-5

VI – Spectroscopy

- **Spectroscopy** (spectrometry & spectrophotometry) is a large and varied group of instrumental techniques in which various types of spectra are produced and analyzed.
- The **types of spectra** include: bright-line emission spectra, mass spectra, infrared-absorption spectra, visible-absorption spectra, ultraviolet-absorption spectra, photoelectron-absorption spectra, microwave-absorption spectra, and nuclear magnetic-absorption spectra.
- **Spectral analysis** give researches the ability to determine the mass, composition, and structure of laboratory samples.

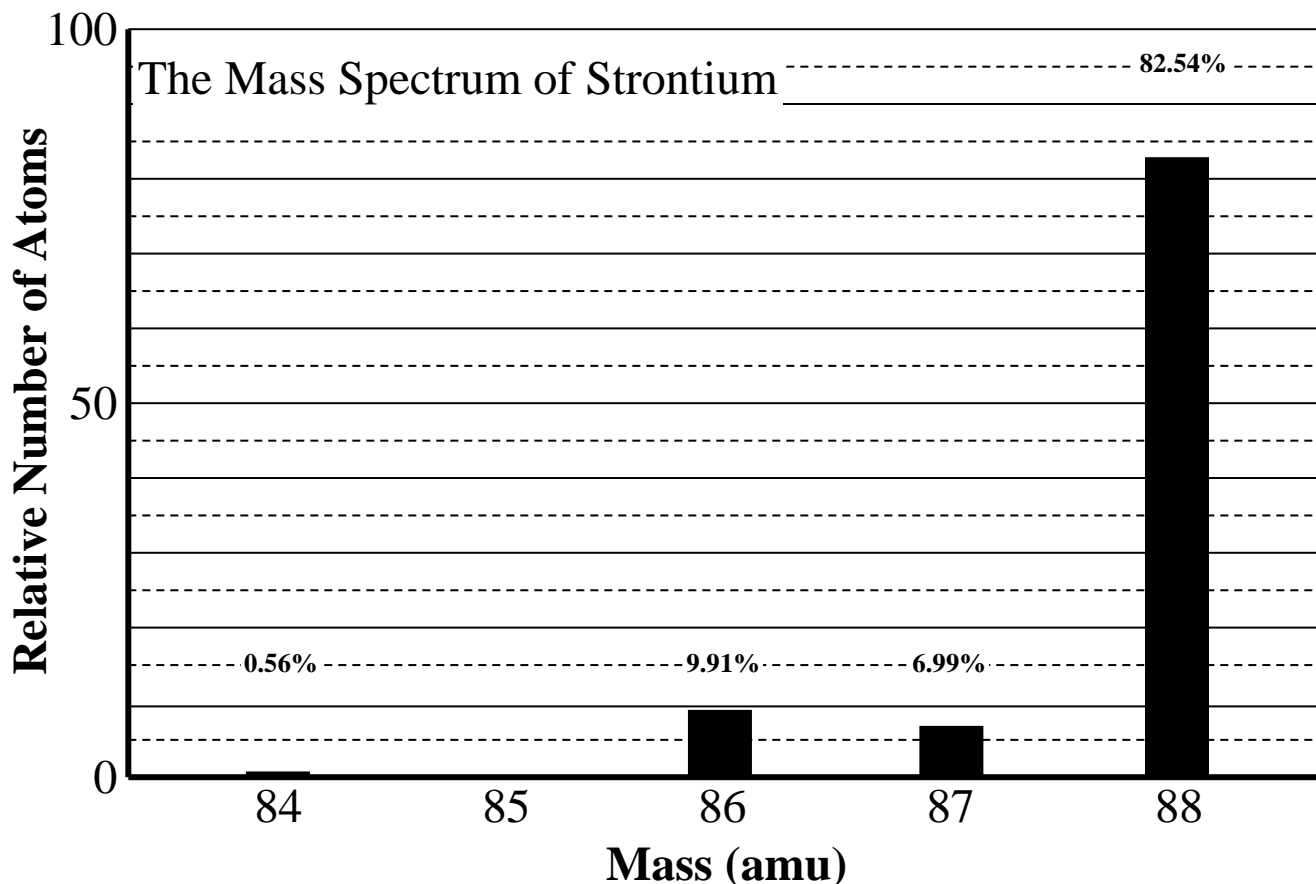
A) Bright-Line Emission Spectroscopy (Consult your 1st year notes.)



- When elements in the gaseous phase are excited by a source of energy, their electrons will absorb exact quanta of energy and then release them in the form of photons. Each released photon produces a characteristic spectral-line at a specific wavelength which can be viewed in a spectroscope. Together they create the element's unique bright-line emission spectrum.

B) Mass Spectrometry (Consult pages 30 – 31 of your summer assignment booklet.)

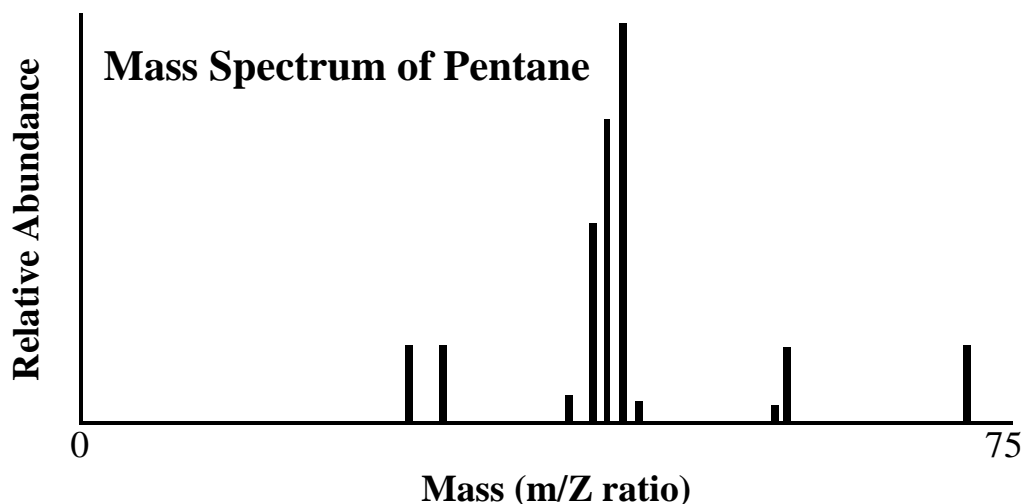
- The average atomic mass for an element can be determined from mass spectrometry data which gives both the masses of the isotopes present as well as their percent abundances.



$$\text{Mass} \approx (0.0056)(84) + (0.0991)(86) + (0.0699)(87) + (0.8254)(88)$$

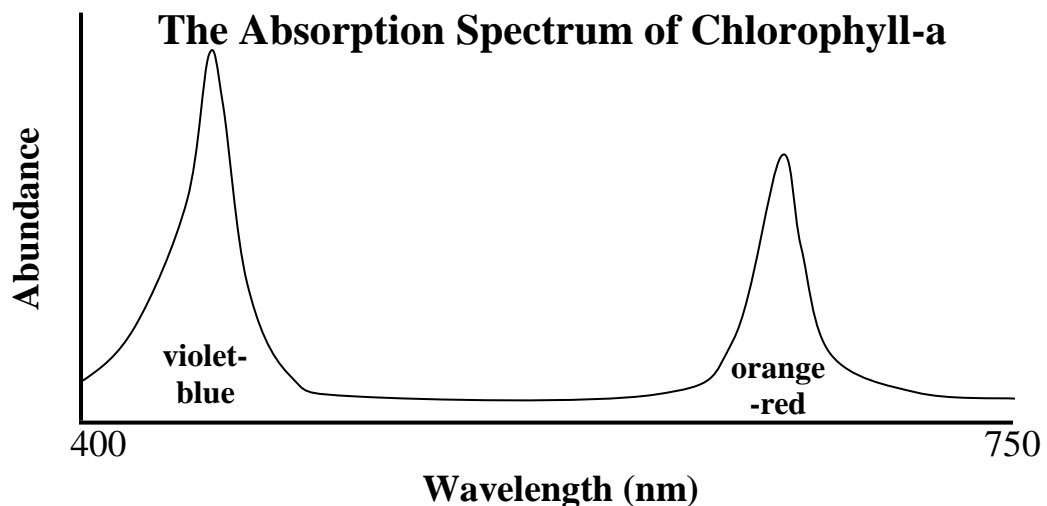
$$\text{Mass} \approx 87.71 \text{ amu (an approximation since actual atomic masses were not used)}$$

- The masses for compounds can also be determined from their mass spectra but their analyses are beyond the scope of this class.

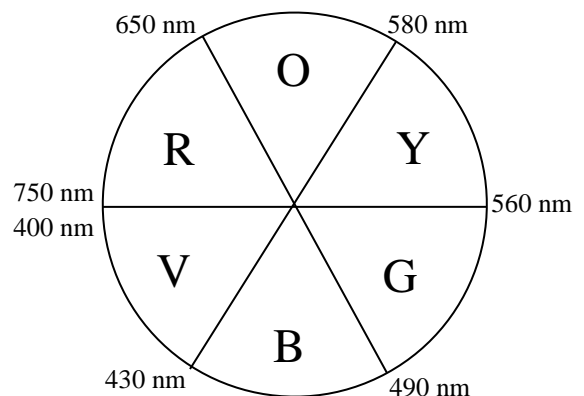


C) Visible and Ultraviolet Absorption Spectroscopy

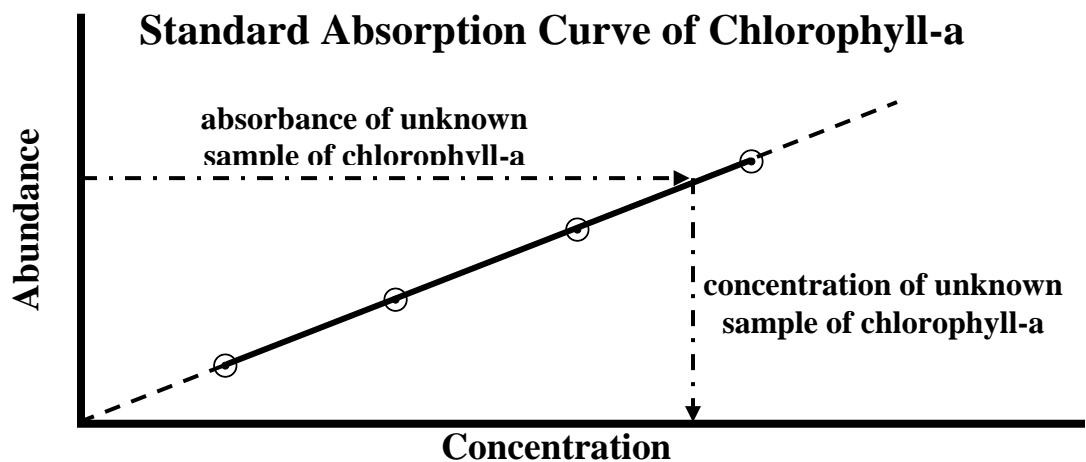
- The electrons in atoms and molecules are able to absorb photons from the visible and ultraviolet regions of the electromagnetic spectrum as they transition to higher energy levels.
- The visible and ultraviolet absorption spectrum is unique for each atom and molecule.
- **Visible absorption spectroscopy** is often used to study **colored** substances, which absorb specific wavelengths from white light.



- The unique visible absorption spectrum of chlorophyll-a, with its characteristic peaks (440 nm & 670 nm) are a means of identifying it from an unknown substance.
- Chlorophyll-a appears greenish in color since it absorbs strongly in the violet-blue and orange-red parts of the visible spectrum.
- A sample has a particular color for one of two reasons:
 - 1) It reflects or transmits light of that color.
 - 2) It absorbs light of the complementary color.
- Complementary colors can be determined by using an artist's color wheel.
- The complementary color of a mixture of violet-blue and orange-red is a greenish color.



- In addition to identifying a substance, absorption spectroscopy can be used to measure how much of a substance is present in an unknown sample such as chlorophyll-a dissolved in ether.
 - 1) Absorbance readings for several solutions of chlorophyll-a of known concentration are made at a specific wavelength using an instrument called a spectrophotometer.
 - 2) The data is then plotted and the resulting graph is known as the standard curve.
 - 3) The absorbance reading for the solution of chlorophyll-a of unknown concentration is taken.
 - 4) Using the standard absorption curve, the concentration of the solution of chlorophyll-a of unknown concentration is made.



- Since the concentration of chlorophyll-a present in the solution is directly related to the amount of light being absorbed, then there exists a mathematical relationship between concentration and absorbance which is known as the Beer-Lambert law:

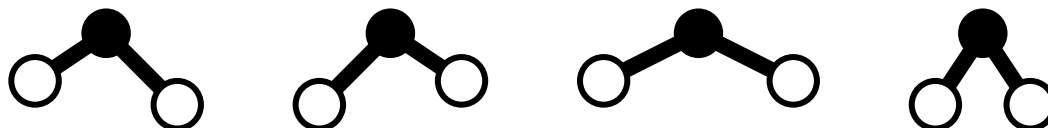
$$A = abc$$

where A is absorbance, a is the molar absorptivity coefficient, b is the path length through which the light traveled, and c is the concentration of the solution.

- The Beer-Lambert law is a " $y = mx + b$ " equation where " y " is A, where " m " is ab, where " x " is c and where " b " is zero which makes sense since a solvent with no solute should not absorb light assuming that the instrument had been properly calibrated to read zero when only the solvent was present.

D) Infrared Absorption Spectroscopy

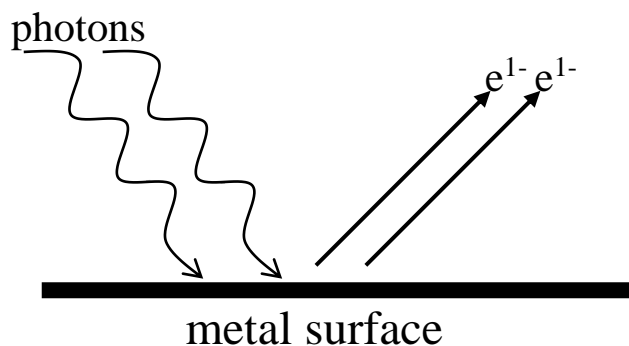
- Photons associated with infrared light are not energetic enough to cause electrons to transition from lower to higher energy states but can induce vibrational excitation of covalently bonded atoms.
- Covalently bonded atoms vibrate about the bond through bending and stretching/compressing motions.



- Like electron excitation, vibrational bond excitation is quantized and thus every covalently bonded substance has a unique infrared absorption spectrum.

E) Photoelectron Spectroscopy (PES)

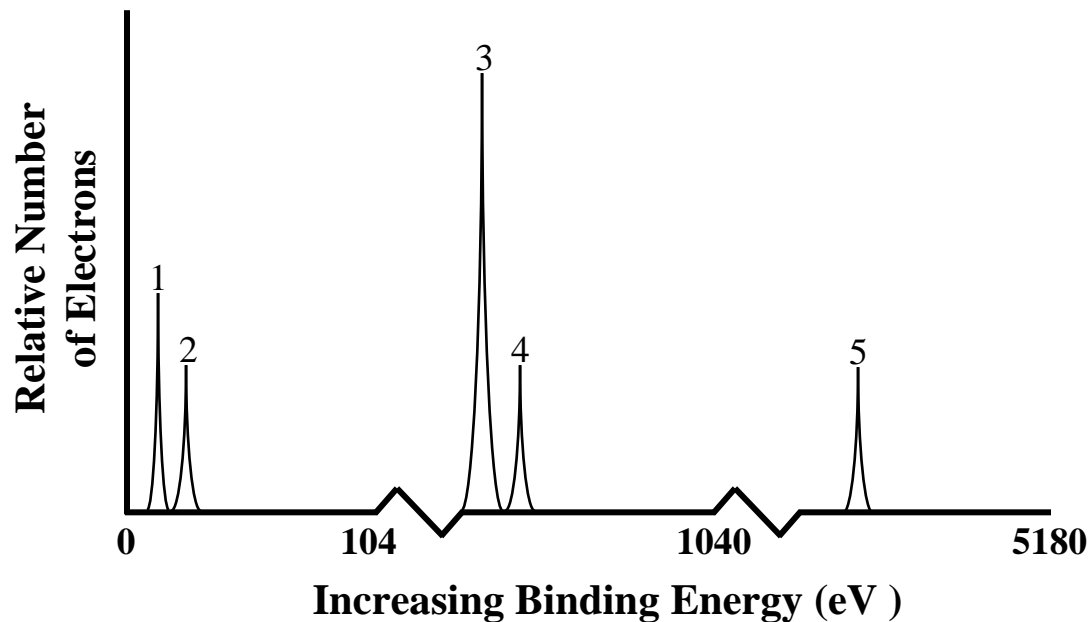
- If an electron in an atom absorbs enough energy, it can leave the atom. An example of this is the photoelectric effect.



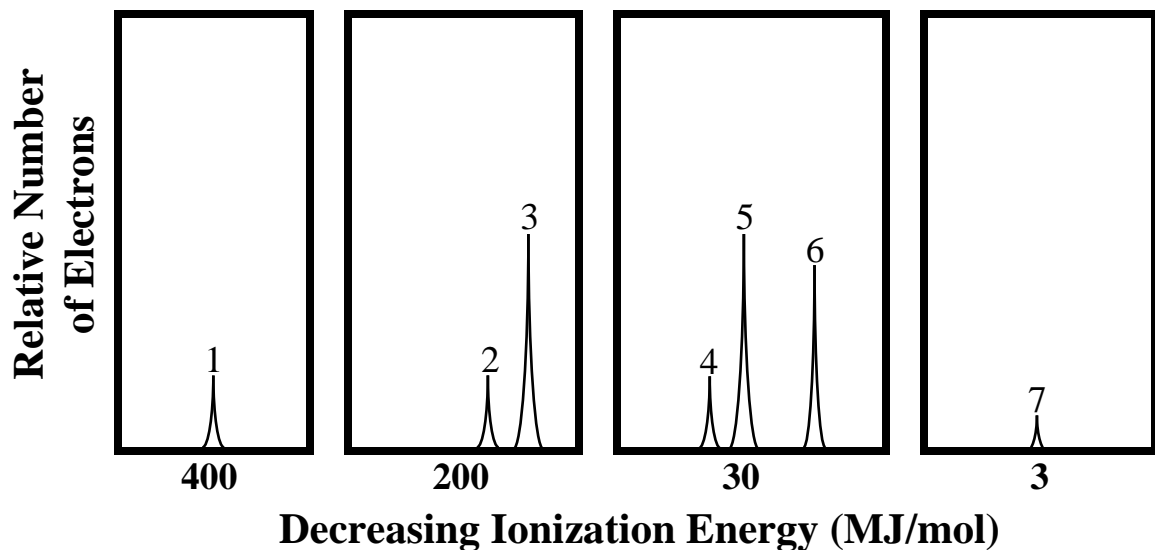
- When an atom loses an electron it becomes a positive ion and the minimum energy required to do this is called the ionization energy.
- Since every atom has a unique electronic structure with unique electron orbital energies, then the energies required to induce the electrons to leave the atom can be used to determine the atom's electron configuration. This technique is called photoelectron spectroscopy (PES).
- The ionization energies (binding energies) measured by photoelectron spectroscopy are usually given in units of **MJ/mole** or **electron volts (eV)**. $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$

- Photoelectron spectra are usually presented in one of two ways.

1) The photoelectron spectrum for phosphorus: (increasing energy)



2) The photoelectron spectrum for chromium: (decreasing energy)



- The binding energy of each peak reveals the orbital energy and the peak intensity reveals the number of electrons in each orbital.

1) The photoelectron spectrum for phosphorus: (read backward)

peak-5: $1s^2$; peak-4: $2s^2$; peak-3: $2p^6$; peak-2: $3s^2$; peak-1: $3p^3$

2) The photoelectron spectrum for chromium: (read forward)

peak-1: $1s^2$; peak-2: $2s^2$; peak-3: $2p^6$; peak-4: $3s^2$;

peak-5: $3p^6$; peak-6: $3d^5$; peak-7: $4s^1$